

Information Dimension of Dissipative Quantum Walks

P. Schijven* and O. Mülken†

Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany

(Dated: August 14, 2014)

We study the temporal growth of the von Neumann entropy for dissipative quantum walks on networks. By using a phenomenological quantum master equation, the quantum stochastic walk (QSW), we are able to parametrically scan the crossover from purely coherent quantum walks to purely diffusive random walks. In the latter limit the entropy shows a logarithmic growth, which is proportional to the information dimension of the random walk on the network. Here we present results for the von Neumann entropy based on the reduced density operator of the QSW. It shows a similar logarithmic growth for a wide range of parameter values and networks. As a consequence, we propose the logarithmic growth rate of the von Neumann entropy to be a natural extension of the information dimension to dissipative quantum systems. We corroborate our results by comparing to numerically exact simulations.

Much effort has been put into understanding dynamical properties of excitation transfer on various networks [1]. Based on the continuous-time quantum walk (CTQW) [2], one of the intriguing questions is if it is possible to achieve a classification of its quantum dynamics, similar to the classical universality classes [3]. For continuous-time random walks (CTRW), this can be done by studying the scaling exponents of dynamical properties such as the mean square displacement, the mean first passage time and the average return probability [4, 5]. Due to the highly oscillatory nature of the CTQW however, many of these exponents do not translate well to the quantum regime [1]. In this letter, we show that this problem can be approached by studying the so-called information dimension associated with a CTQW on a network in a dissipative environment.

For classical random walks on networks, the information dimension is a dynamical exponent which is defined by the logarithmic growth of the entropy [6, 7]. Recently, much interest has been shown in the growth of the (entanglement) entropy in diffusive and disordered systems [8–10]. Additionally, much attention has recently been given to understand the entropy production rate in open quantum systems [11, 12]. In this letter we provide a new perspective on the entropy growth of dissipative quantum walks by relating it to a generalized form of the information dimension.

We first provide the formalism that allows us to describe the (reduced) dynamics of an excitation in an open quantum system/network. When the environmental correlation time is small compared to the relaxation time of the network, one can describe the dynamics (of the reduced density matrix $\rho(t)$) on the network by a master equation in Lindblad form [13]:

$$\frac{d\rho(t)}{dt} = -i[\mathbf{H}_0, \rho(t)] + \sum_{k,l=1}^N \lambda_{kl} \mathcal{D}[\mathbf{L}_{kl}, \rho(t)], \quad (1)$$

where \mathbf{H} is the Hamiltonian of the (closed) system/network of N nodes, where each node k is associated with a basis vector $|k\rangle$ ($k = 1, \dots, N$), all of which

span the accessible Hilbert space for the closed system [1]. The rate constants satisfy $\lambda_{kl} \geq 0$ for all k and l . The dissipator is given by

$$\mathcal{D}[\mathbf{L}_{kl}, \rho(t)] = \mathbf{L}_{kl} \rho(t) \mathbf{L}_{kl}^\dagger - \frac{1}{2} \left\{ \mathbf{L}_{kl}^\dagger \mathbf{L}_{kl}, \rho(t) \right\}, \quad (2)$$

with the Lindblad operators \mathbf{L}_{kl} . Depending on the strength of the coupling to the environment, different types of dynamics can occur. In the case of weak coupling the dynamics is mostly coherent, which we model by CTQW. Following the formalism of the CTQW, the network's Hamiltonian is then chosen to be directly proportional to the connectivity matrix \mathbf{A} of the network: $\mathbf{H}_0 \equiv \mathbf{A}$ [1, 2]. On the other hand, for high temperatures and strong coupling, we assume in what follows that the environment induces incoherent hopping, i.e., a CTRW between the nodes of the network after most coherent signatures are gone [13]. In order to model the CTRW, we utilize the freedom of choosing the set of Lindblad operators \mathbf{L}_{kl} [13]: It can be shown that the Lindblad operator $\mathbf{L}_{mn} = |m\rangle \langle n|$, for $m \neq n$, models an incoherent transition from node $|n\rangle$ to node $|m\rangle$ [14–16]. Following Förster theory or Marcus' theory of electron transport, we can then estimate the incoherent transition rates $k_{n \rightarrow m}$ between the nodes $|n\rangle$ and $|m\rangle$ by using Fermi's golden rule, i.e., $k_{n \rightarrow m} \sim |\langle m | \mathbf{H}_0 | n \rangle|^2$ [17–19]. Upon setting $\lambda_{mn} = k_{n \rightarrow m}$ we obtain the correct CTRW from the dissipator.

We now use the Lindblad equation to construct a phenomenological model that allows us to interpolate between these two limiting scenarios. This model is also known as the Quantum Stochastic Walk (QSW) [14]. The master equation then takes the following form:

$$\begin{aligned} \frac{d\rho_\alpha(t)}{dt} = & (1 - \alpha) \mathcal{L}_{\text{CTQW}}[\rho_\alpha(t)] \\ & + \alpha (\mathcal{L}_{\text{CTRW}}[\rho_\alpha(t)] + \mathcal{L}_{\text{deph}}[\rho_\alpha(t)]) \end{aligned} \quad (3)$$

with $\alpha \in [0, 1]$, $\mathcal{L}_{\text{CTQW}}[\rho_\alpha(t)] = -i[\mathbf{H}_0, \rho_\alpha(t)]$. Furthermore, $\mathcal{L}_{\text{CTRW}}[\rho_\alpha(t)]$ models that part of the dissipator in Eq. (2) which describes the environmentally induced

CTRW, while $\mathcal{L}_{\text{deph}}[\rho_\alpha(t)]$ is that part of the dissipator which induces a localized dephasing process. To model the latter, we choose the (diagonal) Lindblad operators $\mathbf{L}_{mm} = |m\rangle\langle m|$ and, for simplicity, we choose the dephasing rates to be $\lambda_{nn} \equiv \lambda = 1$.

In order to validate our model for more realistic systems, we also use the numerically exact Hierarchy Equations of Motion approach (HEOM) to solve the reduced dynamics of the system [20]. In this method, one attempts to solve the Liouville-von Neumann equation for the full system-environment Hamiltonian \mathbf{H}_{tot} by constructing a hierarchy of auxiliary density matrices. [21] This hierarchy can be truncated and computed efficiently if one assumes that the system-environment interaction is governed by a Lorentzian spectral density [20]: $J(\omega) = (\omega\Omega\Lambda)/[2(\omega^2 + \Omega^2)]$, where Λ is the reorganization energy of the bath and Ω its characteristic response frequency.

Due the Markovian nature of the QSW dynamics, it approaches a thermally mixed stationary state when $t \rightarrow \infty$ [13]. This is reflected by the von Neumann entropy

$$S_{\text{vn}}(t, \alpha) = -\text{tr} \{ \rho_\alpha(t) \ln \rho_\alpha(t) \}, \quad (4)$$

which increases from $S_{\text{vn}}(0, \alpha) = 0$ to its maximal value $\lim_{t \rightarrow \infty} S_{\text{vn}}(t, \alpha) = \ln N$ for all $\alpha > 0$ [13]. Here, we are interested in the question if the growth of $S_{\text{vn}}(t, \alpha)$ can be related to certain scaling exponents associated with the dynamics on the underlying network.

In the classical limit, ($\alpha \rightarrow 1$) $S_{\text{vn}}(t, \alpha)$ reduces to the classical Shannon entropy $H(t)$ of the environmentally induced CTRW:

$$H(t) \equiv \lim_{\alpha \rightarrow 1} S_{\text{vn}}(t, \alpha) = - \sum_k p_{kj}(t) \ln[p_{kj}(t)], \quad (5)$$

where $p_{kj}(t) = \lim_{\alpha \rightarrow 1} \langle k | \rho_\alpha(t) | k \rangle$, given that $\rho_\alpha(0) = |j\rangle\langle j|$. For various networks, it has been numerically shown that $H(t)$ grows linearly with $\ln(t)$ after an initial/transient time t_I . The logarithmic growth rate is now defined as the CTRW variant of the information dimension, i.e., $H(t) \sim d_I \ln t$. We pause to note that this definition is akin to the definition of the information dimension of chaotic systems [22]. For a discrete-time random walk, having performed M steps, it is defined as $d_I = I_M / \ln M$. Here $I_M = - \sum_{k=1}^{S_M} P_k \ln P_k$, with P_k being the probability of visiting the k -th site [6, 7]. Upon taking the limit to the CTRW, this matches our definition.

The existence of a logarithmic growth for CTRW can be shown analytically by assuming that the propagator for the CTRW on a generic complex network can be formulated as a stretched exponential [23], $p_{kj}(t) \sim t^{-d_s/2} \exp(-a\xi_k^\nu)$, where $\xi_k = r_k t^{-d_s/2d_f}$. Here, r_k is the position of the k -th node relative to node j , d_f the fractal dimension and d_s the spectral dimension of the network. The latter is reflected in the scaling behaviour of the probability to return or to remain at the origin,

i.e., $p_{jj}(t) \sim t^{-d_s/2}$ [24]. Substituting this form into the definition of $H(t)$ results in:

$$H(t) = \frac{d_s}{2} \ln t + t^{-\nu d_s/2d_f} \sum_k r_k^\nu p_{kj}(t) \approx \frac{d_s}{2} \ln t. \quad (6)$$

In this case we thus obtain $d_I = d_s/2$

Since the von Neumann entropy is well-defined for all values of α and contains the Shannon entropy $H(t)$ as a limiting case, we now introduce the (possibly α -dependent) information dimension $d_I(\alpha)$ for the QSW in a similar way as above. Provided that $S_{\text{vn}}(t, \alpha)$ grows linearly with $\ln(t)$ for intermediate times, $d_I(\alpha)$ is defined by:

$$S_{\text{vn}}(t, \alpha) \sim d_I(\alpha) \ln(t). \quad (7)$$

Note that for $\alpha = 0$, the system is always in a pure state, resulting in $S_{\text{vn}}(t, \alpha = 0) = 0$ for all t . Therefore it is not possible to define $d_I(\alpha)$ for $\alpha = 0$ in this way.

Since an analytic solution of Eq. (3) is only possible for a few cases and for small systems we proceed with a numerical analysis of two important examples. As prototypes for opposing dynamical behaviors we take the linear chain and the so-called Sierpinski gasket. For the former, the CTQW is more efficient, i.e. faster than the corresponding CTRW, while for the latter the converse is true [1, 25]. The Sierpinski gasket is a deterministic fractal structure where each new generation g is determined by subdividing each triangle into three new sub-triangles [26] such that the number of nodes in generation g is given by $N_g = 3(3^{g-1} + 1)/2$.

Fig. 1 shows the von Neumann entropy as a function of time (in log-lin scale) for different values of α for (a) a line of $N = 100$ nodes and for (b) a Sierpinski gasket of generation $g = 5$ with $N = 123$ nodes. The first thing to notice is that at a given small (transient) time ($t < 1$) the entropy in the CTQW limit is smaller than in the CTRW limit. In order to understand this, we consider a dimer, i.e. a network of only two nodes. It is straightforward to show that for times $t \ll 1$ one obtains $S_{\text{vn}}(t, \alpha) \approx \alpha t - \alpha t \ln(\alpha t)$. A similar result has also been obtained for a slightly different model in Ref. [27].

However, with increasing time, the increase in entropy becomes larger the smaller the value of α . Before the entropy reaches its stationary value, we find the logarithmic scaling for both the line and the Sierpinski gasket. While the scaling region stretches over a rather long period of time for values of $\alpha \geq 0.2$, namely $t \in [10, 100]$ for the line and $t \in [1, 10]$ for the gasket, this region is smaller the smaller the values of α . For $\alpha = 0.1$ and for the finite structures considered here, the scaling regions become very small. We are certain that this issue can be resolved by computing the entropy for a larger chain in order to delay the approach to the equilibrium state. The difference in the time scales for the line and the Sierpinski gasket can be understood when realizing that the

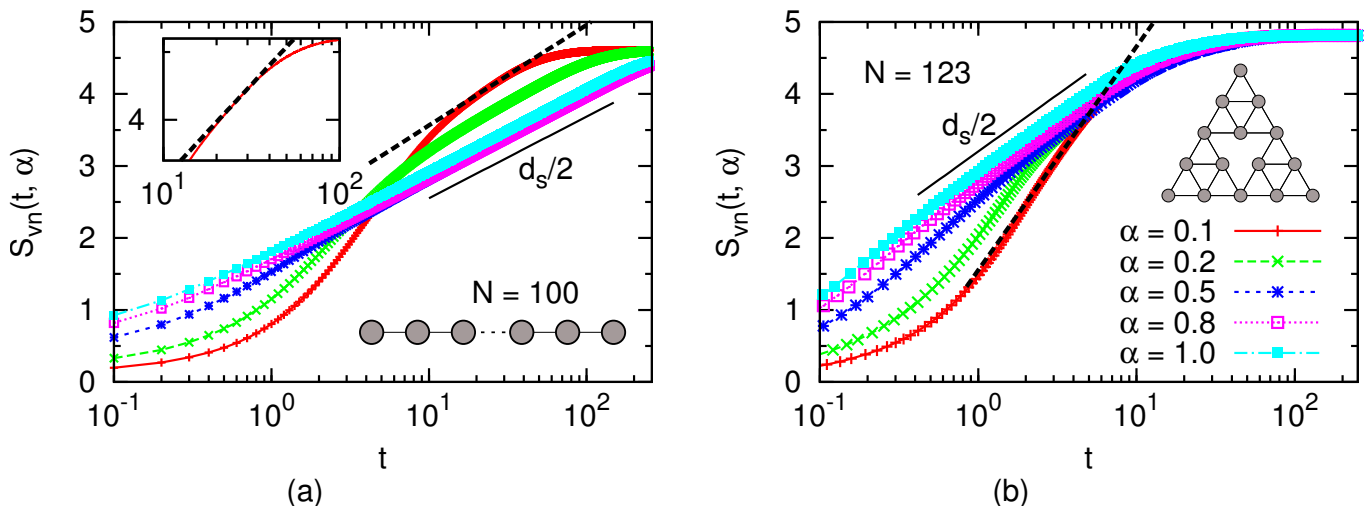


FIG. 1. The left panel (a) shows the von Neumann entropy $S_{\text{vn}}(t, \alpha)$ for a linear chain with $N = 100$ nodes on a log-linear scale for various values of the interpolation parameter α . The right panel (b) shows $S_{\text{vn}}(t, \alpha)$ for a Sierpinski gasket of generation $g = 5$ with $N = 123$ nodes, for the same values of α . In both cases we observe a logarithmic growth regime for most values of α . The dashed black lines illustrate the regions for $\alpha = 0.1$, where we fitted the logarithmic growth regime. The inset in panel (a) shows the fitted result in more detail. The solid black lines illustrate the slopes of the entropy in the classical limit and the illustration of the Sierpinski fractal in the right panel has generation $g = 3$.

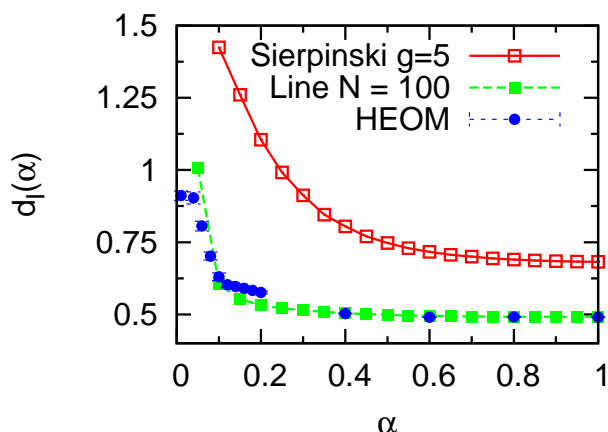


FIG. 2. The information dimension $d_I(\alpha)$ for both the Sierpinski gasket of generation $g = 5$ (red) and the linear chain with $N = 100$ nodes (green). We also show the information dimension $d_I(\Lambda)$ obtained with the HEOM, for a chain of $N = 9$ nodes (blue). We converted $d_I(\Lambda)$ to $d_I(\alpha)$ by choosing $\alpha = \Lambda/500$.

Sierpinski gasket of $g = 5$ has a side length of 17 nodes which is about one order of magnitude smaller than the line with $N = 100$ nodes. A further obvious difference between the two structures is the fact that for the line the entropies for different values cross at times $t \in [1, 10]$ while such a crossing region is far less pronounced for the Sierpinski gasket.

Turning now to the scaling behavior of the entropy,

we find the expected results in the CTRW limit. In this case, the information dimension is determined by the spectral dimension. For the line the spectral dimension is $d_s = 1$ [28]. Thus, for CTRW on a line we obtain $\lim_{\alpha \rightarrow 1} d_I(\alpha) = d_s/2 = 1/2$. The spectral dimension of the Sierpinski gasket is also known [1, 23]: $d_s = 2 \ln 3 / \ln 5 \approx 1.365$. Thus, for CTRW on a Sierpinski gasket we expect $\lim_{\alpha \rightarrow 1} d_I(\alpha) \approx 0.683$, which is larger than the value for the line.

When $\alpha \rightarrow 0^+$, the QSW approaches the CTQW. Recent results for discrete-time quantum walks on periodic one-dimensional lattices suggest that the logarithmic growth of the von Neumann entropy in this limit scales with an exponent which is twice as large as the classical random walk exponent [29]. For our analysis this translates to $\lim_{\alpha \rightarrow 0^+} d_I(\alpha) \approx d_s = 1$.

Fig. 2 shows $d_I(\alpha)$ for the two structures as a function of α . We have extracted the value of $d_I(\alpha)$ from the curves in Fig. 1 by a linear fit in the scaling regions. For both structures we find that $d_I(\alpha)$ increases with decreasing α from 1 to 0.1. For the line the values of $d_I(\alpha)$ remain close to the CTRW value $1/2$ and only start to increase slowly for $\alpha \leq 0.4$, e.g., for $\alpha = 0.1$ we find $d_I(\alpha = 0.1) \approx 0.6$. For smaller values of α there is a steep increase in $d_I(\alpha = 0.1)$ up to values $d_I(\alpha = 0.05) \approx 1$, which is twice as large as the CTRW value. The Sierpinski gasket on the other hand shows a more continuous increase of $d_I(\alpha)$ with decreasing α , e.g., for $\alpha = 0.1$ we find $d_I(\alpha = 0.1) \approx 1.4$, which also is about twice as large as the CTRW value. The fact that for both the line and the Sierpinski gasket, the information dimension is ap-

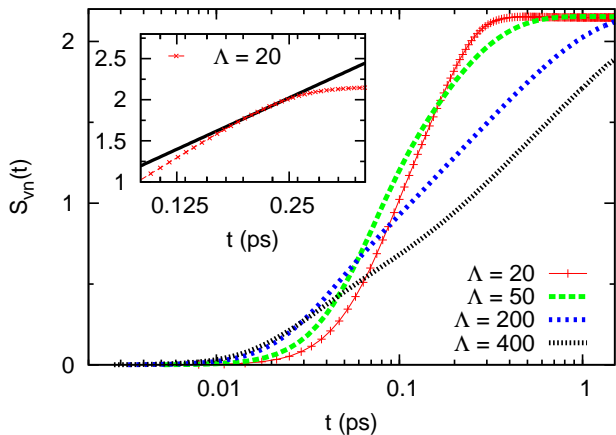


FIG. 3. Log-linear plot showing the von Neumann entropy $S_{\text{vn}}(t)$ obtained with the HEOM for different values of the reorganization energy Λ (in units of cm^{-1}). The inset shows the area for $\Lambda = 20$, where we fitted the logarithmic growth regime.

proximately twice as large in the CTQW regime as in CTRW regime, might indicate that this is a more universal feature which certainly needs further investigation, see also Ref. [29] for the discrete-time quantum walk.

In order to corroborate our findings from our phenomenological model, we also compute the von Neumann entropy $S_{\text{vn}}(t)$ for a linear chain by using the HEOM. To solve the HEOM we use the program PHI [30, 31]. Due to limited computational resources we take a chain of $N = 9$ nodes and truncate the hierarchy at a depth $L = 14$, corresponding to 497420 auxiliary density matrices. In particular, we have $\mathbf{H}_0 = \gamma \mathbf{A}^{\text{line}}$, and choose $\gamma = 50 \text{ cm}^{-1}$ and $\Omega = 35 \text{ ps}^{-1}$. The temperature is chosen to be 300K in order to avoid adding low-temperature Matsubara correction terms to the hierarchy [30, 32, 33]. To obtain classical hopping dynamics for large couplings to the environment we assume a broad spectral density, in accordance with the classical theory of electron transport [17, 19].

In Fig. 3 we show the entropy $S_{\text{vn}}(t)$ computed with the HEOM for various values of the reorganization energy Λ , playing a similar role as the interpolation parameter α for the QSW. Comparing to Fig. 1(a), we observe good overall agreement, including the crossing point for small t , even though the approach toward the scaling regime looks different. This is to be expected since the HEOM allows for a more precise modelling of the dynamics at early times, before most of the coherences have died out. Furthermore, having a small chain introduces finite-size effects that lead to a different form of $S_{\text{vn}}(t)$. Indeed, the inset of Fig. 3, showing the linear fit for $\Lambda = 20 \text{ cm}^{-1}$, has a very small linear regime, making the extraction of the information dimension difficult. Nonetheless, we see in

Fig. 2 that the information dimension $d_I(\Lambda)$ (blue) has a similar shape as the curve for the QSW. For a qualitative comparison to our QSW results, we have converted $d_I(\Lambda)$ into $d_I(\alpha)$ by assuming that $\alpha = \Lambda/500$, since at $\Lambda = 500 \text{ cm}^{-1}$ the dynamics is purely classical, with $d_I(500) = 0.5$. As mentioned before, due to the small size of the chain it was difficult to extract $d_I(\Lambda)$ for small Λ . This is why for small α , the curve in Fig. 2 does not reach the same value of the information dimension as for the QSW.

To conclude, we have seen that the information dimension $d_I(\alpha)$, obtained from the QSW model, is a very useful quantity for classifying the quantum dynamics on networks in dissipative environments, in contrast to earlier methods such as the average return probability. Additionally, the curves for $d_I(\alpha)$ can give insight into the robustness of the quantum dynamics against environmental noise. By comparing to numerically exact computations, we have shown that this result is not sensitive to the particular implementation of the dissipative process, but that it still captures the essential details of the underlying network structure.

We gratefully acknowledge financial support from the Deutsche Forschungsgemeinschaft (DFG grant No. MU2925/1-1) and support from the Deutscher Akademischer Austauschdienst (DAAD grant No. 56266206 and project No. 40018). Furthermore, we would like to thank A. Anischenko and A. Blumen for useful discussions.

* petrus.schijven@physik.uni-freiburg.de

† muelken@physik.uni-freiburg.de

- [1] O. Mülken and A. Blumen, Phys. Rep. **502** (2011).
- [2] E. Farhi and S. Gutmann, Phys. Rev. A **58**, 915 (1998).
- [3] B. D. Hughes, *Random Walks and Random Environments*, Vol. 1 (Oxford University Press, 1995).
- [4] N. van Kampen, *Stochastic Processes in Physics and Chemistry* (North Holland, Amsterdam, 1990).
- [5] S. Havlin and D. Ben-Avraham, Adv. Phys. **51**, 187 (2002).
- [6] P. Argyrakis, Phys. Rev. Lett. **59** (1987).
- [7] N. Pitsianis, G. Bleris, and P. Argyrakis, Phys. Rev. B **39** (1989).
- [8] M. Serbyn, Z. Papić, and D. A. Abanin, Phys. Rev. Lett. **110**, 260601 (2013).
- [9] H. Kim and D. A. Huse, Phys. Rev. Lett. **111**, 127205 (2013).
- [10] J. H. Bardarson, F. Pollmann, and J. E. Moore, Phys. Rev. Lett. **109**, 017202 (2012).
- [11] B. Leggio, A. Napoli, A. Messina, and H.-P. Breuer, Phys. Rev. A **88**, 042111 (2013).
- [12] S. Deffner and E. Lutz, Phys. Rev. Lett. **107**, 140404 (2011).
- [13] H. Breuer and F. Petruccione, *The theory of open quantum systems* (Oxford University Press, 2010).
- [14] J. D. Whitfield, C. A. Rodríguez-Rosario, and A. Aspuru-Guzik, Phys. Rev. A **81**, 022323 (2010).

- [15] P. Schijven and O. Mülken, Phys. Rev. E **85**, 062102 (2012).
- [16] P. Schijven, J. Kohlberger, O. Mülken, and A. Blumen, J. Phys. A: Math. Theor. **45**, 215003 (2012).
- [17] R. A. Marcus, J. Chem. Phys. **24**, 966 (1956).
- [18] T. Förster, Discuss. Faraday Soc. **27**, 7 (1959).
- [19] A. Nitzan, *Chemical Dynamics in Condensed Phases: relaxation, transfer and reactions in condensed molecular systems* (Oxford University Press, 2006).
- [20] Y. Tanimura and R. Kubo, J. Phys. Soc. Jpn **58**, 1199 (1989).
- [21] Here, the environment is modeled in terms of the Caldeira-Leggett model, as a bath of harmonic oscillators that is linearly coupled to the system [34].
- [22] E. Ott, *Chaos in Dynamical Systems* (Cambridge University Press, 1993).
- [23] J. Klafter, G. Zumofen, and A. Blumen, J. Phys. A: Math. Gen. **24**, 4835 (1991).
- [24] S. Alexander and R. Orbach, J. Physique Lett. **43**, 625 (1982).
- [25] E. Agliari, A. Blumen, and O. Mülken, J. Phys. A: Math. Theor. **41**, 445301 (2008).
- [26] See the inset in Fig. 1(b) for an illustration for $g = 3$.
- [27] M. Nizama and M. O. Cáceres, J. Phys. A: Math. Theor **45**, 335303 (2012).
- [28] O. Mülken and A. Blumen, Phys. Rev. E **73**, 066117 (2006).
- [29] B. Kollár and M. Koniorczyk, Phys. Rev. A **89**, 022338 (2014).
- [30] J. Strümpfer and K. Schulten, J. Chem. Theory Comput. **8**, 2808 (2012).
- [31] PHI was developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign.
- [32] A. Ishizaki and Y. Tanimura, J. Phys. Soc. Jpn. **74**, 3131 (2005).
- [33] L. Chen, R. Zheng, Y. Jing, and Q. Shi, J. Chem. Phys. **134**, 194508 (2011).
- [34] A. O. Caldeira and A. J. Leggett, Ann. Phys. **149**, 374 (1983).